Discrimination of leucine and isoleucine via fragmentation by electromagnetic field

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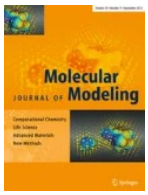

Journal of Molecular Modeling

Aims and scope

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Abstract

Context

We conduct comparative numerical studies of the effects of electric dipole field and electromagnetic radiation field on the amino acids leucine and isoleucine. Since they are structural isomers, distinguishing them by mass is a non-trivial task, while determination of protein structure can be crucial on many occasions. We emphasize the influence of the magnetic field of radiation by utilizing a modified basis sets with correction coefficients to the s— and p— orbitals following the Anisotropic Gaussian Type Orbitals method. Studying the electric potential of the isomers in dipole electric or electromagnetic fields proves that the different layout of leucine vs isoleucine is the main reason why some fragments could not

be formed during chemical bond cleavage. Comparison of the chemical structure of the fragments created due to the decomposition of the isomers in the dipole electric or electromagnetic fields shows that their decomposition products are different. These findings can be used also for discrimination between the two isoleucine conformers, for which the cleavage starts at different values of the dipole electric field strength, as well as the products of the decomposition reaction are not identical. Our numerical calculations of the fragmentation outcomes, taking into account the magnetic field effects, can serve as a guidance for discrimination between the isomers/conformers.

Methods

We applied the Becke's three-parameter hybrid functional approach with non-local correlation by Lee, Yang, and Parr ($B3LYP$), together with the $cc-pVTZ$ basis set as it is implemented in the GAUSSIAN09 quantum chemistry package in order to obtain the most stable conformers of leucine and isoleucine. We used the options provided by GAUSSIAN09 to add finite external field in order to perform the calculations of leucine and isoleucine in the electric dipole and electromagnetic fields. The Anisotropic Gaussian Type Orbitals method was used to obtain the correction coefficients which modify the original $cc-pVTZ$ basis set in order to account for the effects of magnetic field of radiation. Results were visualized and the electrical potentials analyzed by the Molden visualization program.

Availability of data and materials

The data presented in this study are available on request from the corresponding author. The data are not publicly available, due to authors' rights.

Code Availability

Not applicable

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Contributions

J. T. conceptualized the idea of the paper, performed numerical simulations and formal analysis of the data, and wrote the corresponding parts of the paper. T. K. developed the methodology and applied the corresponding models, performed formal analysis of the data, as well as prepared the draft of the paper.

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Ethics declarations

Competing interests

The authors declare no competing interests.

Ethics approval

Not applicable

Consent to participate

Not applicable

Consent for publication

Not applicable

Additional information

Publisher's Note

Appendices

Appendix A: Modified basis set

In this Appendix we show details of the modification of the $cc-PVTZ$ basis set (as it is implemented in the GAUSSIAN09 quantum chemistry package) according to the *AGTO* methodology in order to obtain the basis set functions in the presence of magnetic field. In the GAUSSIAN09 package a single basis function consists of different primitive Gaussian functions of the form [15]:

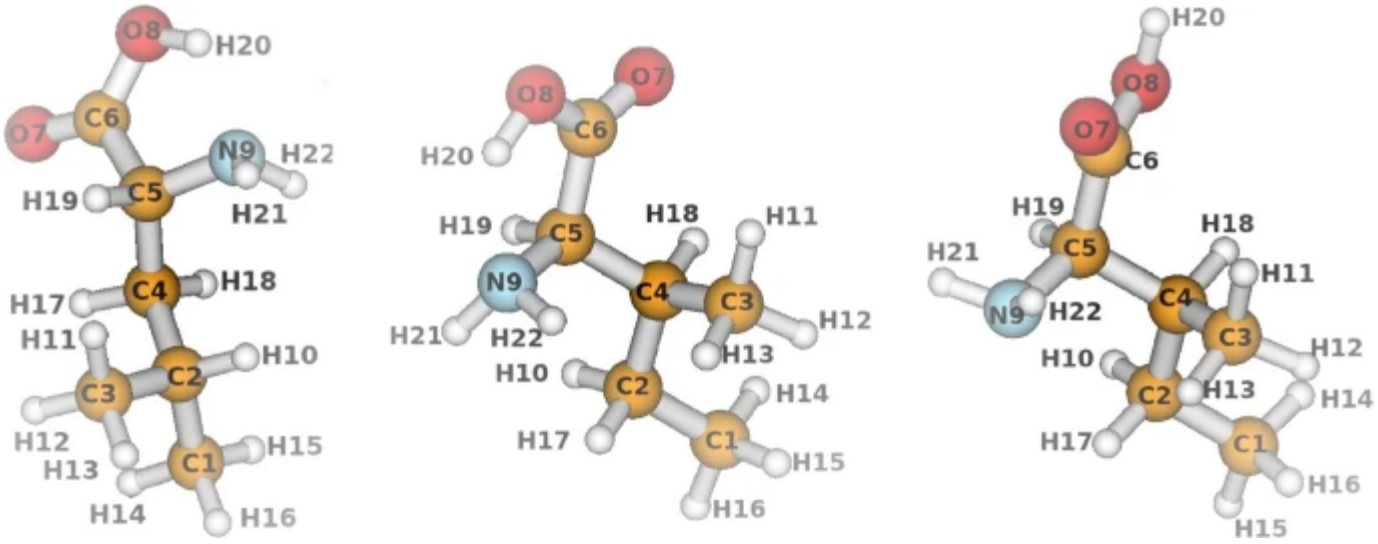
$$\varphi_{\mu}(r)=\sum_{i=1}^{N} d_{i\mu} e^{-\alpha_{i\mu} {f_{\mu}}^{2} r^{2}}, \tag{A.1}$$

where N signifies the number of primitive functions, $d_{i\mu}$ are contraction coefficients, $\alpha_{i\mu}$ are the exponents, while f_μ represent scaling factors. Each shell is described accordingly, for example, the s-shells contain one s-type basis function, the p-shells contain three basis functions (p_x, p_y, p_z), d-shells are defined as five basis functions ($d_{z^2-r^2}$, $d_{x^2-r^2}$, d_{xy}, d_{xz}, d_{yz}), etc. In order to obtain the modified $cc-PVTZ$ basis set, which accounts for the magnetic field effects, we add the correction coefficients $\alpha_1 = \beta_1 = 0.0539737$ (as calculated in Section 2) to the exponents $\alpha_{i\mu}$ in Eq. A.1 of the $s-$ and $p-$orbitals of the C, N, O, and H atoms.

Appendix B: Effects of dipole electric/electromagnetic fields on the molecular bond lengths

In this Appendix we show the bond variations at the dipole electric/ electromagnetic field strengths leading to the decomposition of the compounds. The values of the field strengths are taken from Table 2. Figure 4 shows the numbering of the atoms and the respective bonds in Leu (on the left), Ile1 (in the centre) and Ile2 (on the right). The data presented in Tables 3, 4 and 5 clearly indicates that the distance between the atoms or the molecular fragments (in bold) is higher than that represented in the literature as bond length among the respective atoms (see the main text for the values of the typical $C-C$, $C-O$, $C-H$, and $O-H$ bond lengths).

Fig. 4



Atom numbering and bond notations Leu (on the left), Ile1 (in the centre), and Ile2 (on the right)

Table 3 Bond lengths in Leu without/in the dipole electric and electromagnetic fileds

Table 4 Bond lengths in Ile1 without/in the dipole electric and electromagnetic fileds

Table 5 Bond lengths in Ile2 without/in the dipole electric and electromagnetic fileds

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